

SYSTEM AND METHOD FOR
STRUCTURE-BASED DRUG DESIGN
THAT INCLUDES ACCURATE
PREDICTION OF BINDING FREE ENERGY

Abstract

A system and method for providing improved *de novo* structure-based drug design that includes a method for more accurately predicting binding free energy. The system and method use a coarse-graining model with corresponding knowledge-based potential data to grow ligand candidates and libraries of ligand candidates. In light of the present inventions using the coarse-graining model, the novel growth method of the present invention uses a metropolis Monte Carlo selection process which result in a low energy structure that is not necessarily the lowest energy structure, yet results in a better ligand candidate.